Quantum mechanics in general quantum systems (IV): Green operator and path integral

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We first rewrite the perturbation expansion of the time evolution operator [An Min Wang, quant-ph/0611216] in a form as concise as possible. Then we derive out the perturbation expansion of the time-dependent complete Green operator and prove that it is just the Fourier transformation of the Dyson equation. Moreover, we obtain the perturbation expansion of the complete transition amplitude in the Feynman path integral formulism, and give an integral expression that relates the complete transition amplitude with the unperturbed transition amplitude. Further applications of these results can be expected and will be investigated in the near future.

PACS numbers: 03.65.-w, 03.65.Ca

I. INTRODUCTION

The study on quantum mechanics in general quantum systems is still progressing. Recently, we have obtained the exact solution [1], perturbation theory [2] and open systems dynamics [3] in general quantum systems. However, a whole theoretical formulism requires us to investigate more problems and obtain more conclusions. We continue our endeavor in this paper.

As is well-known, it is convenient and general to study and express quantum mechanics in the operator form as possible using Dirac symbol system [4]. This requires us to rewrite our results in such a concise form. Actually, it is helpful to study on the formal theory of quantum mechanics in general quantum systems. This is the first task and the starting point in this paper.

After the exact solution [1] and perturbation theory [2] of quantum mechanics in general quantum systems, we should consider the Green operator (function) [5] and the Feynman transition amplitude (propagator) of path integral [6] because many physical conclusions can be expressed and calculated by them. Actually, the Green function approach provides a unified systematic method for calculating various quantities of physical interest. The path integral formulism builds a formal frame for more complicated quantum theory, for example, quantum field theory and quantum statistics, and gives a relatively easy road to expressions for Greens functions, which are closely related to amplitudes for physical processes such as scattering and decays of particles.

Whatever Green operator or path integral, their calculations are not simple in general when the concerned systems are complicated. Hence, from the view of perturbation theory, we would like to obtain their perturbation expansion for general quantum systems in order to avoid the difficulty and carry out related calculations. At present, this is a known effective way to deal with quantum mechanics in general and complicated quantum systems. When we focus our attention on the time evolution of the systems, it will be very useful to extend Dyson equation [7, 8] about the time-independent (stationary) Green operator (function) to one about the time-dependent (dynamical) Green operator (function), that is, to derive out an explicit perturbation expansion of the time-dependent complete Green operator (function). Here, the time-independent Green function means that it is a solution to the stationary Schrödinger equation with the point resource, while the time-dependent Green function means that it is a solution to the dynamical Schrödinger equation with the point resource. Moreover, it is very interesting to find the explicit perturbation expansion of the Feynman transition amplitude (propagator) with the path integral form in general quantum systems. Furthermore, we expect to relate the complete transition amplitude to the unperturbed transition amplitude. This must be able to provide a way to calculate the path integral expression of the transition amplitude even the concerned systems are complicated. In addition, the two perturbation expansions include all order approximations of perturbation and have a known general term, they should be able to play an important role in the formal study of quantum theory.

This paper is organized as the following: in this section, we give an introduction; in Sec. II, we rewrite the perturbation expansion of the time evolution operator [1] in the form as concise as possible; in Sec. III, we derive

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out the perturbation expansion of the time-dependent complete Green operator and prove that it is just a Fourier transformation of the Dyson equation; in Sec. IV, we obtain the perturbation expansion of the complete transition amplitude in the Feynman path integral formulism, and give an integral expression that relates the complete transition amplitude with the unperturbed transition amplitude; in Sec. V, we give some discussions and summarize our conclusions.

II. PERTURBATION EXPANSION OF THE TIME EVOLUTION OPERATOR

In our recent paper [1], we obtain the general and explicit expression of the time evolution operator (for simplicity, set $\hbar = 1$)

$$\mathrm{e}^{-\mathrm{i}Ht} = \sum_{l=0}^{\infty} \mathcal{A}_l(t) = \sum_{l=0}^{\infty} \sum_{\gamma,\gamma'} A_l^{\gamma\gamma'}(t) |\Phi^\gamma\rangle \left\langle \Phi^{\gamma'} \right| \tag{1}$$

where the Hamiltonian H has been written as the summation of the unperturbed H_0 and the perturbing Hamiltonian H_1. While $A_l^{\gamma\gamma'}(t)$ are defined by

$$A_0^{\gamma\gamma'}(t) = \mathrm{e}^{-\mathrm{i}E_\gamma t}\delta_{\gamma\gamma'} \tag{2}$$

$$A_l^{\gamma\gamma'}(t) = \sum_{\gamma_1,\cdots,\gamma_{l+1}} \left[\sum_{i=1}^{l+1} (-1)^{i-1} \frac{\mathrm{e}^{-\mathrm{i}E_{\gamma_i}t}}{d_i(E[\gamma,l])}\right] \left[\prod_{j=1}^{l} H_1^{\gamma_j\gamma_{j+1}}\right] \delta_{\gamma_1\gamma}\delta_{\gamma_{l+1}\gamma'}. \tag{3}$$

where $H_1^{\gamma_i\gamma_{i+1}} = \langle \Phi^{\gamma_i}|H_1|\Phi^{\gamma_{i+1}}\rangle$ are called the perturbing Hamiltonian matrix elements, $|\Phi^\gamma\rangle$ is the eigenvector of H_0 and E_γ is the corresponding eigenvalue, that is

$$H_0|\Phi^\gamma\rangle = E_\gamma|\Phi^\gamma\rangle, \tag{4}$$

and the denominators $d_i(E[\gamma,l])$ in $A_l^{\gamma\gamma'}(t)$ reads

$$d_1(E[\gamma,l]) = \prod_{i=1}^{l} \left(E_{\gamma_1} - E_{\gamma_{i+1}}\right), \tag{5}$$

$$d_i(E[\gamma,l]) = \prod_{j=1}^{i-1} \left(E_{\gamma_j} - E_{\gamma_i}\right) \prod_{k=i+1}^{l+1} \left(E_{\gamma_i} - E_{\gamma_k}\right), \tag{6}$$

$$d_{l+1}(E[\gamma,l]) = \prod_{i=1}^{l} \left(E_{\gamma_i} - E_{\gamma_{l+1}}\right), \tag{7}$$

where $2 \le i \le l$. The expression of the time evolution operator (1) is both a c-number function and a power series of the perturbation. Therefore, it is useful and effective for the calculation of perturbation theory. However, it is not convenient for the study on the formal theory of quantum theory. In order to overcome this shortcoming, we, using the Dirac symbol formulism, first rewrite the $\mathcal{A}$ in the following form

$$\mathcal{A}_l(t) = \sum_{i=1}^{l+1} \sum_{\gamma_i} \left(G_{0E_{\gamma_i}} H_1\right)^{i-1} \mathrm{e}^{-\mathrm{i}H_0 t} |\Phi^{\gamma_i}\rangle\langle\Phi^{\gamma_i}| \left(H_1 G_{0E_{\gamma_i}}\right)^{l+1-i} \tag{8}$$

where $G_{0E_{\gamma_i}}$ is the unperturbed Green operator defined by

$$G_{0E_{\gamma_i}} = \frac{1}{E_{\gamma_i} - H_0} \tag{9}$$

or more strictly, it is the restarted or advanced unperturbed Green operator defined by

$$G_{0E_{\gamma_i}}^{(\pm)} = \frac{1}{E_{\gamma_i} - H_0 \pm \mathrm{i}\epsilon} \tag{10}$$

where $\epsilon \to 0^+$ [8] and E_{γ_i} take over all of eigenvalues of H_0. Note that we cannot write the expression of the time evolution operator in a full operator form independent of the representation because its perturbation expansion depends on the spectrum of the unperturbed Hamiltonian. Substituting (8) into (1), we have the concise form of the time evolution operator

$$\mathrm{e}^{-\mathrm{i}Ht} = \sum_{l=0}^{\infty}\sum_{i=1}^{l+1}\sum_{\gamma_i}\left(G_{0E_{\gamma_i}}^{(\pm)}H_1\right)^{i-1}\mathrm{e}^{-\mathrm{i}H_0 t}|\Phi^{\gamma_i}\rangle\langle\Phi^{\gamma_i}|\left(H_1 G_{0E_{\gamma_i}}^{(\pm)}\right)^{l+1-i} \tag{11}$$

III. PERTURBATION EXPANSION OF THE TIME-DEPENDENT COMPLETE GREEN OPERATOR

In quantum mechanics, the Green operator (or function) plays a very important role, for example, in the perturbation theory. It is a kernel of the integral form of the Schrödinger equation, in special, the Lippmann-Schwinger equation [9]. It is clear that we have

$$\left[E_\gamma - H_0\right] G_{0E_\gamma}^{(\pm)} = 1 \tag{12}$$

Or in the representation of localized coordinate bases, the corresponding Green function $G_{0E_\gamma}^{(\pm)}(\boldsymbol{x},\boldsymbol{x}') = \langle\boldsymbol{x}|G_{0E_\gamma}^{(\pm)}|\boldsymbol{x}'\rangle$ obeys the stationary Schröding equation with the point resource, i.e

$$\left[E_\gamma - H_0(\boldsymbol{x},-\mathrm{i}\boldsymbol{\nabla}_{\boldsymbol{x}})\right] G_{0E_\gamma}^{(\pm)}(\boldsymbol{x},\boldsymbol{x}') = \delta(\boldsymbol{x}-\boldsymbol{x}') \tag{13}$$

Here, we called it as the time-independent (stationary) unperturbed Green function in order to distinguish the time-dependent (dynamical) unperturbed Green function that obeys the following dynamical Schröding equation with the point resource:

$$\left[\mathrm{i}\frac{\partial}{\partial t} - H_0(\boldsymbol{x},-\mathrm{i}\boldsymbol{\nabla}_{\boldsymbol{x}})\right] G_0^{(\pm)}(\boldsymbol{x},\boldsymbol{x}';t,t') = \delta(t-t')\delta(\boldsymbol{x}-\boldsymbol{x}') \tag{14}$$

Similarly, the time-independent complete Green function and the time-dependent complete Green function satisfy, respectively

$$\left[E_\gamma - H(\boldsymbol{x},-\mathrm{i}\boldsymbol{\nabla}_{\boldsymbol{x}})\right] G_{E_\gamma}^{(\pm)}(\boldsymbol{x},\boldsymbol{x}') = \delta(\boldsymbol{x}-\boldsymbol{x}') \tag{15}$$

$$\left[\mathrm{i}\frac{\partial}{\partial t} - H(\boldsymbol{x},-\mathrm{i}\boldsymbol{\nabla}_{\boldsymbol{x}})\right] G^{(\pm)}(\boldsymbol{x},\boldsymbol{x}';t,t') = \delta(t-t')\delta(\boldsymbol{x}-\boldsymbol{x}') \tag{16}$$

It is easy to obtain the time-independent complete Green operator

$$G_{E_\gamma}^{(\pm)} = \frac{1}{E_\gamma - H \pm \mathrm{i}\epsilon} \tag{17}$$

Moreover, the time-independent complete Green operator (or function) can be given by the Dyson equation

$$G_{E_\gamma}^{(\pm)} = G_{0E_\gamma}^{(\pm)} + G_{0E_\gamma}^{(\pm)} H_1 G_{E_\gamma}^{(\pm)} = G_{0E_\gamma}^{(\pm)}\sum_{l=0}^{\infty}\left(H_1 G_{0E_\gamma}^{(\pm)}\right)^l \tag{18}$$

It is actually the perturbation expansion of the time-independent complete Green operator. Just well-known, the time-dependent Green operator is the Fourier transformation of the time-independent Green operator, that is

$$G_0^{(\pm)}(t,t') = \frac{1}{2\pi}\int_{-\infty}^{\infty}\mathrm{d}E_\gamma G_{0E_\gamma}^{(\pm)}\mathrm{e}^{-\mathrm{i}E_\gamma(t-t')} \tag{19}$$

$$G^{(\pm)}(t,t') = \frac{1}{2\pi}\int_{-\infty}^{\infty}\mathrm{d}E_\gamma G_{E_\gamma}^{(\pm)}\mathrm{e}^{-\mathrm{i}E_\gamma(t-t')} \tag{20}$$

Obviously, it is difficult to calculate this integral when we directly substitute the Dyson equation (18) into the above relation. In other words, ones have not yet clearly known its explicit form, that is, a perturbation expansion with the

factors of primary functions of time so far. However, using the concise form of the time evolution operator (11), we can derive out it.

Actually, this derivation is easy from the relation between the time-dependent complete Green operator and the time evolution operator

$$G^{(+)}(t,t') = -\mathrm{i}\theta(t-t')\mathrm{e}^{-\mathrm{i}H(t-t')} \tag{21}$$
$$G^{(-)}(t,t') = \mathrm{i}\theta(t'-t)\mathrm{e}^{-\mathrm{i}H(t-t')} \tag{22}$$

This immediately yields

$$G^{(+)}(t,t') = -\mathrm{i}\theta(t-t')\sum_{l=0}^{\infty}\sum_{i=1}^{l+1}\sum_{\gamma_i}\left(G^{(+)}_{0E_{\gamma_i}}H_1\right)^{i-1}\mathrm{e}^{-\mathrm{i}H_0(t-t')}|\Phi^{\gamma_i}\rangle\langle\Phi^{\gamma_i}|\left(H_1G^{(+)}_{0E_{\gamma_i}}\right)^{l+1-i} \tag{23}$$
$$G^{(-)}(t,t') = \mathrm{i}\theta(t'-t)\sum_{l=0}^{\infty}\sum_{i=1}^{l+1}\sum_{\gamma_i}\left(G^{(-)}_{0E_{\gamma_i}}H_1\right)^{i-1}\mathrm{e}^{-\mathrm{i}H_0(t-t')}|\Phi^{\gamma_i}\rangle\langle\Phi^{\gamma_i}|\left(H_1G^{(-)}_{0E_{\gamma_i}}\right)^{l+1-i} \tag{24}$$

Now, let us prove the above perturbation expansion of the time-dependent complete Green operator be a Fourier transformation of the Dyson equation (18). In other words, the inversion transformation of Eq. (23) is just the Dyson equation (18).

From the relations

$$-\mathrm{i}\int_{-\infty}^{\infty}\mathrm{d}t\;\theta(t-t')\mathrm{e}^{-\mathrm{i}H_0(t-t')}\mathrm{e}^{\mathrm{i}E_\gamma(t-t')} = G^{(+)}_{0E_\gamma} \tag{25}$$
$$\mathrm{i}\int_{-\infty}^{\infty}\mathrm{d}t\;\theta(t'-t)\mathrm{e}^{-\mathrm{i}H_0(t-t')}\mathrm{e}^{\mathrm{i}E_\gamma(t-t')} = G^{(-)}_{0E_\gamma} \tag{26}$$

it follows that

$$\begin{aligned}G^{(\pm)}_{E_\gamma} &= \int_{-\infty}^{\infty}\mathrm{d}t\;G^{(\pm)}(t,t')\mathrm{e}^{\mathrm{i}E_\gamma(t-t')}\\ &= \sum_{l=0}^{\infty}\sum_{i=1}^{l+1}\sum_{\gamma_i}\left(G^{(\pm)}_{0E_{\gamma_i}}H_1\right)^{i-1}G^{(\pm)}_{0E_\gamma}|\Phi^{\gamma_i}\rangle\langle\Phi^{\gamma_i}|\left(H_1G^{(\pm)}_{0E_{\gamma_i}}\right)^{l+1-i}\\ &= -\sum_{l=0}^{\infty}\sum_{\gamma,\gamma'}\sum_{\gamma_1,\cdots,\gamma_{l+1}}\left[\sum_{i=1}^{l+1}(-1)^{i-1}\frac{1}{d_i^{(\pm)}(E[\gamma,l])(E_{\gamma_i}-E_\gamma\mp\mathrm{i}\epsilon)}\right]\left[\prod_{j=1}^{l}H_1^{\gamma_j\gamma_{j+1}}\right]\delta_{\gamma_1\gamma}\delta_{\gamma_{l+1}\gamma'}|\Phi^\gamma\rangle\left\langle\Phi^{\gamma'}\right|\end{aligned} \tag{27}$$

where $d_i^{(\pm)}(E[\gamma,l])$ is defined by adding $\pm\mathrm{i}\epsilon$ to its every factor of the energy level difference.

Based on the appendix in our previous paper [1], if we set $E_\gamma = E_{\gamma_{l+2}} \mp 2\mathrm{i}\epsilon$, we have $d_i(E[\gamma,l])(E_{\gamma_i}-E_{\gamma_{l+2}}) = d_i(E[\gamma,l+1])$. Again using our identity [1]

$$\sum_{i=1}^{l+1}(-1)^{i-1}\frac{E^K_{\gamma_i}}{d_i(E[\gamma,l])} = \begin{cases}0 & (\text{If } 0\le K<l)\\ 1 & (\text{If } K=l)\end{cases}\quad. \tag{28}$$

we obtain

$$G^{(\pm)}_{E_\gamma} = G^{(\pm)}_{0E_\gamma} + \sum_{l=1}^{\infty}\sum_{\gamma,\gamma'}\sum_{\gamma_1,\cdots,\gamma_{l+1}}(-1)^{l+1}\left.\frac{1}{d^{(\pm)}_{l+2}(E[\gamma,l+1])}\right|_{E_{\gamma_{l+2}}=E_\gamma\pm 2\mathrm{i}\epsilon}\left[\prod_{j=1}^{l}H_1^{\gamma_j\gamma_{j+1}}\right]\delta_{\gamma_1\gamma}\delta_{\gamma_{l+1}\gamma'}|\Phi^\gamma\rangle\left\langle\Phi^{\gamma'}\right| \tag{29}$$
$$= G^{(\pm)}_{0E_\gamma}\sum_{l=0}^{\infty}\left(H_1G^{(\pm)}_{0E_\gamma}\right)^l = G^{(\pm)}_{0E_\gamma} + G^{(\pm)}_{0E_\gamma}H_1G^{(\pm)}_{E_\gamma} \tag{30}$$

Therefore, we finish our proof. This implies that the perturbation expansion (23) of the time-dependent complete Green operator, as the Fourier transformation of the Dyson equation (18), is obtained by using the concise form of the time evolution operator (11).

IV. PERTURBATION EXPANSION OF THE COMPLETE TRANSITION AMPLITUDE

Path integral is a formulism that yields the quantum-mechanical amplitudes in a global approach involving the properties of a system at all times. From our perturbation expansion of the time evolution operator, we can see that the time-dependent parts for every term in the summation (11) are expressed in a factor $\exp(-\mathrm{i}H_0 t)$. Hence, only to find the path integral expression of $\exp(-\mathrm{i}H_0 t)$ can keep the features and advantages of the path integral formula.

Here, for simplicity, we assume the space to be one-dimensional. Thus, the unperturbed transition amplitude $K_0(x_b,t_b;x_a,t_a)$ and the complete transition amplitude $K(x_b,t_b;x_a,t_a)$ $(t_b > t_a)$ are defined, respectively, by

$$K_0(x_b,t_b;x_a,t_a) \;=\; \langle x_b|\mathrm{e}^{-\mathrm{i}H_0(t_b-t_a)}|x_a\rangle \tag{31}$$

$$K(x_b,t_b;x_a,t_a) \;=\; \langle x_b|\mathrm{e}^{-\mathrm{i}H(t_b-t_a)}|x_a\rangle \tag{32}$$

From Eq. (11) it immediately follows that the perturbation expansion of the complete transition amplitude

$$K(x_b,t_b;x_a,t_a) = \sum_{l=0}^{\infty}\sum_{i=1}^{l+1}\sum_{\gamma_i}\int \mathrm{d}y_b\mathrm{d}y_a \langle x_b|\left(G^{(\pm)}_{0E_{\gamma_i}}H_1\right)^{i-1}|y_b\rangle K_0(y_b,t_b;y_a,t_a)\langle y_a|\Phi^{\gamma_i}\rangle\langle\Phi^{\gamma_i}|\left(H_1 G^{(\pm)}_{0E_{\gamma_i}}\right)^{l+1-i}|x_a\rangle \tag{33}$$

In fact, this is an integral expression that relates the complete transition amplitude with the unperturbed transition amplitude, that is

$$K(x_b,t_b;x_a,t_a) = \int \mathrm{d}y_b\mathrm{d}y_a C(x_b,y_b;x_a,y_a)K_0(y_b,t_b;y_a,t_a) \tag{34}$$

where

$$C(x_b,y_b;x_a,y_a) = \sum_{l=0}^{\infty}\sum_{i=1}^{l+1}\sum_{\gamma_i}\langle x_b|\left(G^{(\pm)}_{0E_{\gamma_i}}H_1\right)^{i-1}|y_b\rangle\langle y_a|\Phi^{\gamma_i}\rangle\langle\Phi^{\gamma_i}|\left(H_1 G^{(\pm)}_{0E_{\gamma_i}}\right)^{l+1-i}|x_a\rangle \tag{35}$$

If the path integral expression of $K_0(x_b,t_b;x_a,t_a)$ has been found as follows [6, 10]

$$K_0(x_b,t_b;x_a,t_a) = A\int_{x(t_a)=x_a}^{x(t_b)=x_b}\mathcal{D}x\mathrm{e}^{\mathrm{i}\mathcal{S}_0[x]} \tag{36}$$

where A and $S_0[x]$ are known, while

$$\int \mathcal{D}x = \lim_{N\to\infty}\prod_{n=1}^{N}\mathrm{d}x_n \tag{37}$$

Substituting Eq. (36) into Eq. (34), we can rewrite the integral expression (34) as

$$K(x_b,t_b;x_a,t_a) = A\int \mathrm{d}y_b\mathrm{d}y_a C(x_b,y_b;x_a,y_a)\int_{y(t_a)=y_a}^{y(t_b)=y_b}\mathcal{D}y\mathrm{e}^{\mathrm{i}\mathcal{S}_0[y]} \tag{38}$$

This implies that, if the unperturbed transition amplitude $K_0(x,t;x',t')$ is known, then the complete transition amplitude can be obtained in principle even the concerned system is complicated. However, for practical purposes, the cut-off approximation is possible to be required, and finding the above integral analytically might not be a simple task. Perhaps, the numerical method has its playing role.

Obviously, the extension of the above conclusions to three dimensional space is direct.

V. CONCLUSION AND DISCUSSION

In this paper, we first rewrite the perturbation expansion of the time evolution operator in a more concise form than Ref. [1]. Since this expansion depends on the whole spectrum of the unperturbed Hamiltonian, it cannot be written as a full operator form independent of the representation. But, this concise form (11) indeed has been approximatively expressed as the operator form. In terms of it, we also can rewrite our exact solution. Such a form can be used to the our future study on the formal theory of quantum mechanics in general quantum systems.

Then we derive out the perturbation expansion of the time-dependent complete Green operator. It is difficult to obtain directly by the definitions (19) and (20) and the Dyson equation. Moreover, we prove that it is a Fourier transformation of Dyson equation. It is worthy pointing out that the general term of this perturbation expansion has been found and all order approximation of perturbation is included. Just like the case that Dyson equation has extensive applications, we think that our perturbation expansion of the time-dependent complete Green operator will have corresponding interesting applications in the quantum theory, in special, in the problems about the transition probability and the formal scattering.

In the last, we obtain the perturbation expansion of the complete transition amplitude in the Feynman path integral formulism, and give an integral expression that relates the complete transition amplitude with the unperturbed transition amplitude. In fact, this expansion will not only be able to simplify the calculation of path integral in some quantum systems but also can provide a kind of way, at least the probability, to obtain the expression of path integral for general quantum systems. Although the result is an infinite series, it can be cut-off since this series is a power series of perturbation. For practical calculation, we are sure that this expansion can produce the significant physical conclusions, at least via the numerical methods. In addition, it may be interesting to study the relation between our perturbation expansion of the transition amplitude and the variational perturbation expansion of the transition amplitude [10]. However, since our perturbation expansion provides a general term for any order approximation, it should have its obvious advantages. It is clear that our integral expression that relates the complete transition amplitude with the unperturbed transition amplitude is helpful to formally studies on quantum theory since it includes all order approximations of perturbation in a tidy and explicit form.

At present, we mainly focus on our attention to try to build the theoretical formulism of quantum mechanics in general quantum systems. Limited by our time and capability, we will delay to study the concrete applications to the near future.

Acknowledgments

We are grateful all the collaborators of our quantum theory group in the Institute for Theoretical Physics of our university. This work was funded by the National Fundamental Research Program of China under No. 2001CB309310, and partially supported by the National Natural Science Foundation of China under Grant No. 60573008.

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